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Installation Restoration Research Program

Conceptual Model and Process Descriptor Formulations for Fate and Transport of UXO

by James M. Brannon, Patrick Deliman, Carlos Ruiz, Cynthia Price, Mohammed Qasim, WES

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Prepared for Headquarters, U.S. Army Corps of Engineers

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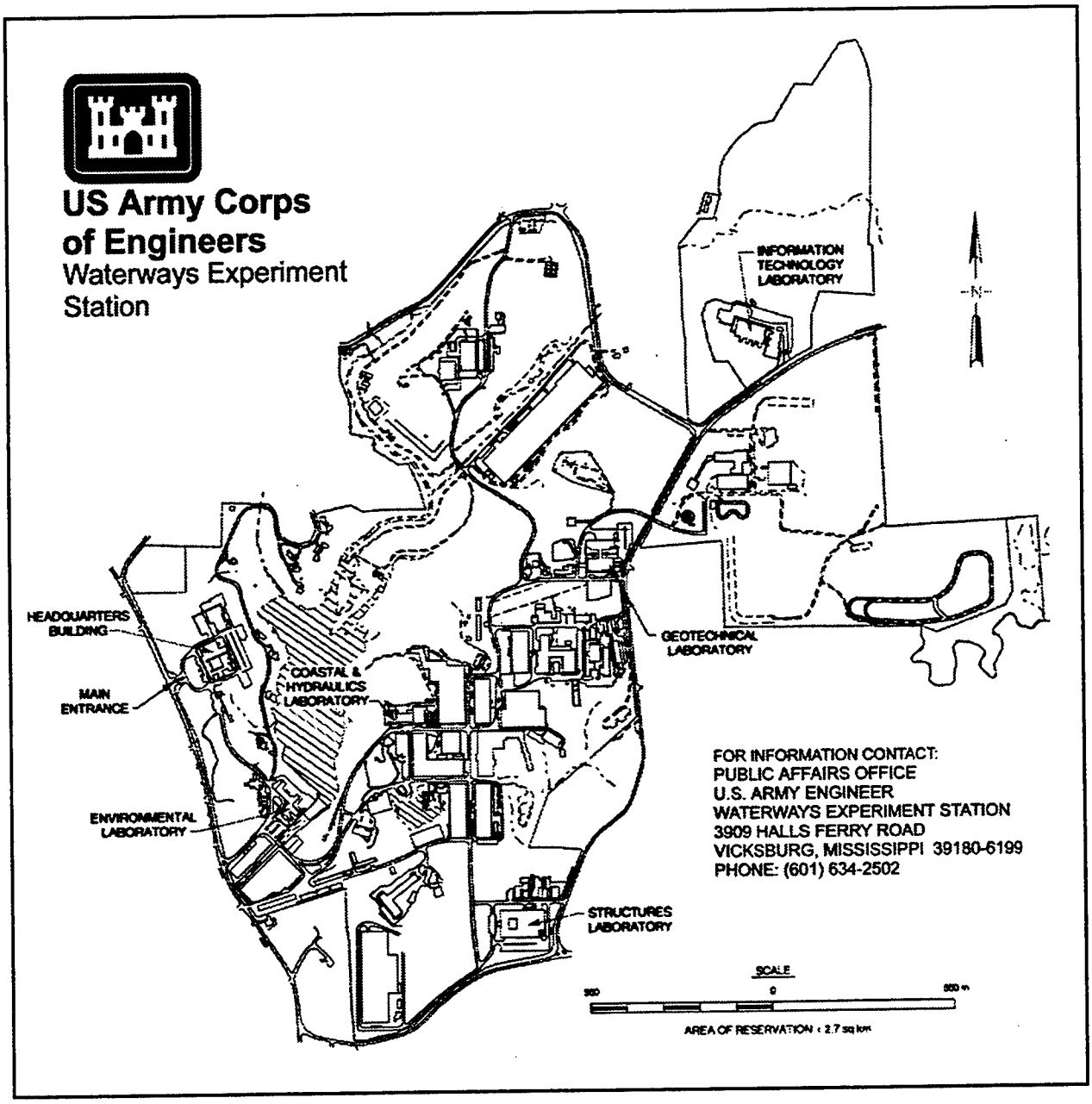

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Preface

The work reported herein was conducted by the U.S. Army Engineer Waterways Experiment Station (WES) for Headquarters, U.S. Army Corps of Engineers (HQUSACE). Funding was provided by the HQUSACE Installation Restoration Research Program (IRRP), Fate & Effects Thrust Area, Work Unit entitled Fate and Transport of Unexploded Ordnance (UXO). Dr. Clem Myer was the IRRP Coordinator at the Directorate of Research and Development, HQUSACE. The IRRP Program Manager was Dr. M. John Cullinane.

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1 Introduction

Unexploded Ordnance (UXO) is military munitions that have been prepared for action, fired, dropped, or buried, and remains undetonated, posing a hazard to operations, personnel, or material. The 1997 UXO Clearance Report to Congress estimates that millions of acres throughout the United States, including 1900 Formerly Used Defense Sites (FUDS) and 130 Base Realignment and Closure (BRAC) installations, potentially contain UXO. Implementation of the "Range Rule," which will identify the process for evaluating appropriate response actions on Closed, Transferred, and Transferring Military Ranges, will potentially add millions of additional acres to the UXO cleanup liability for the Army.

A relatively large body of information exists on explosives concentrations at sites impacted by manufacturing operations (Walsh et al. 1993), but little information is available on explosives concentrations from UXO at firing ranges. Fate and transport of explosives from UXO have been identified as a high priority user requirement and as an important emerging need during promulgation of the "Range Rule." Limited research has been conducted in this area and processes controlling the fate and transport of explosives from UXO are poorly understood. Once explosives from UXO move beyond the confines of the delivery system (mortar shell, artillery shell, rocket, etc.), the processes affecting fate and transport should be similar to those associated with explosives contamination from other sources (Brannon and Myers 1997; Townsend and Myers 1996, McGrath 1995). The primary difference in fate and transport of UXO explosives compared to contamination associated with loading, assembling, or packing facilities is the integrity of the delivery system, the transport of explosives from the munition, and the environment (aquatic, terrestrial, wetland, etc.) in which the delivery system comes to rest.

The objective of this report is to present a conceptual model developed for the fate and transport of UXO explosives, identify the most important processes affecting fate and transport of explosives from UXO, and summarize process descriptor formulations applicable to UXO. Research results on adsorption of HMX and photodegradation of TNT in aquatic systems are integrated into this report.

2 Conceptual Models

Conceptual models were developed for different environments where UXO could come to rest after firing. These environments included surface soil, the deep unsaturated (vadose) zone, the saturated zone, surficial sediment, deep sediment, and surface water. Common to all of the models presented is the dissolution process, which, in conjunction with the surface area of exposed explosive and the moisture regime to which the UXO is subjected, governs the movement of explosives from the UXO and into the surrounding environment. The most important process descriptors relevant to the fate and transport of explosive compounds from UXO are those that describe the movement of explosives from the munition to the environment. Explosives contained within UXO are usually in solid form which remains relatively immobile until dissolution occurs.

The corrosion and rupture release mechanisms combined with the various types of UXO that may be encountered in the field pose unique development considerations for the design of a model to simulate the fate and transport of UXO within the environment. The Framework for Risk Analysis and Management of Environmental Systems (FRAMES) (Gene Whelan, personal communication)[1] modeling environment/interface developed by Pacific Northwest National Laboratory operated by Battelle for the Department of Energy will be used as the framework to build the screening level models based on the conceptual models presented here. FRAMES is a modeling environment that allows visualization of the conceptual model and selection of appropriate models to achieve the desired predictive capability. FRAMES allows various modules to be linked together in an object oriented manner. FRAMES contains modules for risk assessment which allow for a complete site assessment and risk exposure analysis.

Many of the processes affecting the fate and transport of explosives in the environment after the explosives are in soil or sediment have previously been reported (Phelan and Webb 1997; McGrath 1995; Townsend and Myers 1996, Brannon and Myers 1997). The development of process descriptors to

[1] Personal communication, 23 May 1998, Gene Whelan, Pacific Northwest National Laboratory, Richland, WA.

characterize the movement of explosives from UXO into the environment are under development and are discussed in more detail in Chapter 4.

Conceptual models for the various environments where UXO can become lodged are very similar in the processes that will affect the fate and transport of UXO explosives. For some conceptual models, a greater number of processes are operative than for others. However, the source term differs in each of the soil and aquatic environments and is discussed as a function of munition type, integrity, composition, and environment. Chapter 3 includes a more detailed discussion of the soil and aquatic environments.

Fate and Transport Processes

The fate and transport processes that act upon UXO depend upon the environment in which the UXO exists and the manner in which it has breached its delivery containment system. The fate and transport processes believed most applicable to explosives from UXO are shown in Figure 1. This figure groups the fate and transport processes by the environment in which the UXO may come to rest.

The processes referred to in Figure 1 are defined by McGrath (1995). The mathematical formulations for these processes can be found in McGrath (1995) and Deliman and Gerald (in publication). The following are short descriptions of the processes referred to in Figure 1.

Advection	The passive movement of a solute with flowing water.
Dispersion	The general term applied to the observed spreading of a solute plume and generally attributed to hydrodynamic dispersion and molecular diffusion.
Adsorption/desorption	The dynamic process by which dissolved, chemical species accumulate (adsorption) at an interface or are released from the interface (desorption) into solution.
Diffusion	The net migration of solute molecules from regions of higher concentration to regions of lower concentration.
Biotic transformation	The modification of a chemical substance in the environment by a biological mechanism.
Oxidation/Reduction	Reactions in which electron(s) are transferred between reactants. The reactant losing an electron(s) is oxidized, while the reactant gaining an electron(s) is reduced.
Covalent binding	The formation of chemical bonds with specific functional groups in soil organic solids.

Polymerization	The process by which the molecules of a discrete compound combine to form larger molecules with a molecular weight greater than that of the original compound, resulting in a molecule with repeated structural units.
Photolysis	The chemical alteration of a compound due to the direct or indirect effects of light energy.
Infiltration	The process by which water enters the soil at the ground surface and moves into deeper horizons.
Evapotranspiration	The collective processes of evaporation of water from water bodies, soil and plant surfaces, and the transport of water through plants to the atmosphere.
Plant root uptake	The transport of chemicals into plants through the roots.
Sedimentation	The removal from the water column of suspended particles by gravitational settling.

Soil

Conceptual models are presented for the fate and transport of explosives from UXO within the surface soil, deep unsaturated zone, and the saturated zone. The surface soil is that part of the soil profile from the ground surface down to a typical depth of 100 cm. The deep unsaturated zone is below the surface soil down to the beginning of the water table. The saturated zone is that area of the soil which resides totally within the water table. Figure 2 illustrates these various soil zones.

Explosives from corroded, leaking, or ruptured UXO munitions in surface soil will be affected by the processes indicated in the conceptual model (Figure 3). The primary source of explosives is the UXO itself, which may have been acted upon by some primary release mechanism (corrosion, leaking, or rupture of the containment system). Once the UXO containment system has been breached, then dissolution of the explosive occurs. In the case of rupture of certain UXO types, the explosive may exist as free product in the soil due to spillage or may be partially contained within the delivery system. After dissolution of the explosive has begun, fate and transport processes interact with the dissolved contaminant. These fate and transport processes include advection, dispersion, adsorption/desorption, diffusion, biotic transformation, oxidation/reduction, covalent binding, polymerization, photolysis, infiltration, evapotranspiration, and plant root uptake.

The conceptual model for fate and transport of explosives from UXO in the deep unsaturated and saturated zones are similar to the model for the surface soil (Figure 3). Fate and transport processes are fewer for the deep unsaturated soil zone than for the surface soil (Figure 1), with photolysis and evapotranspiration processes inactive in the deeper soil zone. The conceptual model for the saturated soil zone is similar to the deep unsaturated zone model with the exception that plant root uptake is assumed to be nonexistent (Figure 1).

The conceptual models for the various soil zones, from the surface soils to the saturated zone, are very similar. The biggest difference among the conceptual models is that the processes affecting fate and transport of explosives decrease as the UXO comes to reside deeper in the soil zones. UXO at a site potentially exists in all of the soil zones simultaneously, depending upon the depth of groundwater.

Sediment

Conceptual models are presented for the fate and transport of explosives within the surficial sediment and deep sediment layers. The surficial sediment is the uppermost layer of sediment of an aquatic environment, typically the first 10 cm of sediment. The deep sediment layer typically begins 10 cm below the surface of the sediment (Figure 4). The conceptual model for fate and transport of explosives from UXO in the surficial and deep sediment zones are similar to the surface soil conceptual model (Figure 3). The processes that act upon explosives from UXO in the surficial and deep sediment are given in Figure 1.

UXO within the surficial sediment environment may be released through corrosion (e.g., pinholes), rupture (e.g., cracks in the delivery system), or leaking through screw threads linking the fuse assembly to the main charge (Darrach, Chutfian, and Plett 1998). If the delivery system containment has been ruptured, then explosive compounds may be spilled over the area (free product in the sediment), and/or explosives may reside partially contained within the delivery system. This release scenario primarily depends on the type of UXO. Once the explosive has been released, dissolution occurs and the explosive is readily available to be acted upon by the fate and transport processes of advection, dispersion, adsorption/desorption, diffusion, biotic transformation, and oxidation/reduction (Figure 1).

The conceptual model for the deep sediment layer is much the same as that presented for surface sediment, except that advection and dispersion from the overlying water (Figure 1) should not be active processes in the deeper sediment. As was the case for soils, UXO is expected to exist simultaneously in both the surface and deep sediment. The source term will differ from that in soils because the explosive from the UXO will be continuously exposed to water rather than on an intermittent basis as is the case for surface and deep unsaturated soils.

Surface Water

Surface water contaminated with explosives from a corroded, ruptured, or leaking UXO can be anticipated to behave as in the conceptual model for soil shown in Figure 3. The primary release mechanisms for the explosives in the UXO are from corrosion, ruptures, and leaking. Depending upon the type of UXO and its design, explosives may have been released directly to the surface water upon impact and/or may reside partially contained within the remains of the delivery system. Once the explosive compounds have breached the delivery system, the process of dissolution allows the explosives to be acted upon by the fate and transport processes of advection, dispersion, adsorption/desorption, diffusion, biotic transformation, photolysis, sedimentation, oxidation/reduction, and evapotranspiration (Figure 1).

3 Source Term

Accurate estimation of the source term is one of the most difficult problems to overcome in describing the fate and transport of explosives from UXO. The movement of explosives from UXO and the subsequent transport and fate of the explosives depends to a great extent upon the type and physical integrity of the munitions following impact on the firing range. The environment in which the UXO comes to rest will also strongly affect the fate and transport of explosives because of the pronounced impact that such conditions have on explosives (Price, Brannon, and Hayes 1997; Price, Brannon, and Yost 1998). Much more data on explosives are available for soils than for sediments. Even in the absence of UXO, explosives exhibit large short-range spatial heterogeneity in surface soils (Jenkins et al. 1997). Over a distance of 61 cm, the concentration of TNT varied by over 26 orders of magnitude (Jenkins et al. 1997). The presence of UXO and the various means by which explosives from UXO are added to the environment can be expected to add to the heterogeneity.

UXO Integrity

UXO can exist on firing ranges in a number of physical states that greatly affect the fate and transport of explosives contained in the UXO. Intact delivery systems may occur at the firing range from either deliberate burial or fired munitions that failed to detonate. Explosives contamination from intact delivery systems results from corrosion and development of pinhole cracks that may occur over time or leaking through screw threads linking the fuse assembly to the main charge. Incomplete detonation or breakup of the delivery system without detonation may also occur, leading to the survival of part or all of the explosive. This explosive may be scattered over the firing range as free product or partially encased in the remains of the delivery system. This results in a complex source term that is not amenable to simple evaluation. Rather than the soil and water concentration being the source as in manufacturing and packing operations, the source term is a function of the flux of explosives from the exposed surface area of free product in addition to the mobilization of soil explosives. The explosives mass flux is, in turn, affected by the exposure to moisture and the dissolution rate of the exposed explosive.

Corrosion is a complex process whose rate varies as a function of the presence and activities of microorganisms (McNeil and Odom 1992), which is in turn influenced by environmental conditions. Transport of explosives from corroded UXO is a more complex process than flux of explosive from the main charge through pinhole perforations in the munitions casing. Corrosion of steel casings will produce a complex local environment comprising intact steel and iron oxidation and reduction products through which the explosives must pass to exit the munition and enter the environment. Recent studies have shown that zero valent iron (McGrath, personal communication,[1] Singh, Comfort, and Shea 1998) and reduced iron (Brannon, Price, and Hayes 1998) can strongly impact the fate and transport of explosives. TNT exposed to zero valent iron disappears from solution rapidly as does RDX, although apparently at a lower rate (McGrath, personal communication).[1] TNT is rapidly removed from solution by reduced iron in the presence of a sorbing surface (Brannon, Price, and Hayes 1998). The reduction processes observed for zero valent iron and reduced iron should be operative for explosives exiting corroded UXO and will greatly impact formulation of the source term. These processes should act to greatly reduce the flux of primary explosives from UXO, possibly producing transformation products that are susceptible to microbial mineralization or sequesteration by soil and sediment organic matter or minerals. The effects of corroded steel on explosives fate and transport will be investigated to determine the rate and extent of these processes on the explosives source term.

The physical integrity of UXO in the aquatic environment affects sediment explosives concentrations. Sampling and analysis of sediment obtained around UXO at Halifax Harbor, Canada, were conducted 50 years after a series of explosions hurled munitions into the harbor. UXO that appeared intact gave low-level signatures of TNT and 2,4-dinitrotoluene (2,4-DNT), the only two explosives compounds tested, while UXO that had been cracked open during the explosion gave no detectable signatures (Darrach, Chuffian, and Plett 1998). Lack of signatures from the cracked UXO was probably a result of its long residence time in the aquatic environment, which resulted in dissolution and dispersion of the explosive. Explosives loss from intact UXO through leaking screw threads is apparently still occurring at Halifax Harbor. This is indicated by the presence of TNT, which is rapidly transformed to other compounds under a wide range of conditions (Price, Brannon, and Hayes 1997). The movement of explosives from UXO in such a scenario should be controlled primarily by diffusion.

Central to either screening level or more comprehensive modeling of the fate and transport of explosives from UXO are methods for gauging the integrity of UXO at various types of firing ranges. This information is imperative for estimating the amount of mobile explosives from UXO that exists at a site. To provide tools for evaluating the integrity of UXO for the source term, field information on the integrity of UXO from antitank rockets, mortars, and artillery

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[1] Personal Communication, 11 September 1998, Chris McGrath, Research Physical Scientist, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.

are being gathered in this study. This information will be used to develop statistical indices for estimating the surface area of exposed explosives and the soil concentration in the vicinity of a point target, which are common for both direct and indirect fire missions. This information, in conjunction with the rainfall regime, dissolution rate of explosives, soil concentrations, and explosives distribution will be used in the source term codes to give planning level estimates of explosives fate and transport from UXO.

Munitions Type

The types of munitions used at a firing range affect the fate and transport of explosives. For example, unexploded antitank rockets at firing ranges were in many cases sheared open through contact with the target. This resulted in spreading of explosives over the soil surface and a residue of explosives in the remaining rocket casing (Jenkins et al. 1997; 1998). The source of explosives from antitank rocket sites are, therefore, primarily on the soil surface, comprising free product in the rocket casings and explosives in the soil. Measured soil HMX concentrations at an antitank rocket range were highest near the target and decreased as distance from the target increased (Jenkins et al. 1997; 1998), presumably through scattering of explosives from sheared rockets. The concentrations of HMX also showed a decrease in concentration with increasing soil depth. These results indicate that for antitank firing ranges, explosives concentrations should be highest near the impact point and decrease with distance from the point target (Jenkins et al. 1997; 1998). The source term includes fluxes from free product contained in sheared and cracked rockets plus soil concentrations from scattered explosives.

At the antitank site, the concentration ratio of HMX:TNT in the soil differed by orders of magnitude from the 70 percent HMX:30 percent TNT in the octol formulation contained in the antitank rocket. Concentrations of TNT in the soil were very low, probably due to photodegradation of the parent compound and/or transformation or immobilization. TNT transformation products were found in the soil at levels consistent with concentrations expected from the TNT in the octol explosive (Jenkins et al. 1997; 1998). This indicates that the composition of the explosive can change from that contained in the munition before significant transport from the source can occur and will greatly affect the formulation of the source term. Changes are much more probable for TNT than for HMX or RDX.

Other munitions will probably behave differently and result in different source terms than for antitank rockets. The source term for mortar and artillery munitions, for example, will comprise surface and subsurface contamination from explosives contained in UXO. This results because the mortar and artillery munitions possess stronger cases and greater earth penetration ability than thin-shelled antitank rockets. Artillery is generally used for indirect fire support instead of direct fire for the antitank rockets which affects the angle at which the munitions strike the target or the soil, greatly affecting their soil penetration. Unexploded mortar and artillery munitions should have more of the explosives

below the soil surface, which precludes photodegradation that affects TNT from antitank rockets.

Environmental Conditions

Army firing ranges are most often located in upland or partially flooded areas. This results in various redox and moisture conditions and different availability of the explosive to the surrounding environment. These phenomena are site specific and will be addressed in the section on process descriptor formulations.

4 Process Descriptor Formulations

Dissolution

The dissolution rate of explosives from free product spilled over the soil or sediment or contained in cracked or partially fragmented munitions is one of the main processes affecting fate and transport of explosives from UXO. Soils analysis has shown concentration gradients for HMX and TNT that are consistent with different rates of dissolution into aqueous solution and kinetic limitations on solubilization (Jenkins et al. 1997). Such limitations have led to the continued presence of free product in soil surface layers decades after contamination occurred. Preliminary studies in completely stirred aqueous systems examining the rate of dissolution of TNT, RDX, and HMX show pronounced differences in water soluble concentrations over time (Jenkins and Miyares, personal communication).[1] Explosives mass change in water was normalized to a first approximation of surface area to obtain flux rates. Surface area was approximated by assuming that the mass of explosive added to the completely stirred systems, 5.81 mg HMX, 5.72 mg RDX, and 5.45 mg TNT, existed as a single cubic crystal of the explosive. The flux of TNT from the solid phase to the liquid phase was much more rapid than that observed for HMX and RDX. Flux rates obtained by linear regression were 4,164 $\mu g\ cm^{-2}\ hr^{-1}$ for TNT, 454 $\mu g\ cm^{-2}\ hr^{-1}$ for HMX, and 360 $\mu g\ cm^{-2}\ hr^{-1}$ for RDX (Table 1). Dissolution flux also depends upon the contact time with water, which can vary with different environments ranging from rainfall events in upland soils to constant contact if exposed to flowing water.

Adsorption Coefficients

Adsorption of explosives by soils and sediments can slow the transport of explosives contaminants from UXO. This is especially important for RDX and HMX, compounds that do not undergo sequestration to any great extent in soils

[1] Personal Communication, 3 December 1997, Thomas Jenkins and Paul Miyares, Research Chemists, U.S. Army Engineer Cold Regions Research & Engineering Laboratory, Hanover, NH.

(Price, Brannon, and Yost 1998). Sequestration of TNT and its transformation products will be most pronounced in soils and sediment high in organic carbon (Price, Brannon, and Hayes 1997; Pennington et al. 1995).

TNT

TNT distribution coefficients ranging from 0.04 to 11 L/kg have been observed in soils with widely different characteristics (Table 2). Pennington and Patrick (1990) showed good correlation between TNT K_d values and soil Fe, cation exchange capacity (CEC), and percent clay content. Evaluation of an expanded number of soils (Table 2) showed that TNT K_d was strongly correlated with CEC ($r^2 = 0.67$). Inclusion of clay and total organic carbon (TOC) in the regression did not improve the fit of the line. Soil Fe concentration was not available for most of the soils evaluated. Using only soil CEC, TNT K_d can be estimated using the following equation.

$$TNT\ K_d = 0.055\ CEC + 1.26 \quad (1)$$

This relationship will overestimate the TNT K_d observed in aquifer soils such as those from Louisiana Army Ammunition Plant (LAAP) (Table 2). The y intercept of 1.26 is much higher than the K_d for the LAAP aquifer soils (Table 2). Attempts to separate the data into high and low organic carbon regimes did not improve the regression coefficient (r^2) or the predictive equation. Equation 1 should be most useful in surface soils where TNT K_d values are generally higher than 1.26 L/kg (Pennington and Patrick 1990). Estimating K_d for aquifer materials with low CEC and TOC is more problematic and may involve assumption of a very low value (<1 L/kg) for initial evaluations.

RDX

RDX distribution coefficents ranging from 0.12 to 3.5 L/kg have been observed for a wide range of soil characteristics (Table 3). This range of K_d's was much lower than that observed for TNT. Evaluation of RDX K_d versus CEC, TOC, and percent clay (Table 3) showed strong correlation with CEC ($r^2 = 0.734$). Inclusion of clay and TOC in the regression did not improve the fit of the line. RDX K_d can be estimated for both surface and aquifer soils using the following equation:

$$RDX\ K_d = 0.056\ CEC + 0.15 \quad (2)$$

HMX

HMX distribution coefficients determined in this study (Appendix A) and other studies ranged from 0.089 to 17.7 L/kg for a wide range of soil characteristics (Table 4). None of the soil characteristics were good predictors of

HMX K_d, either singly or in combination. In the absence of tools for estimating HMX K_d from soil properties, the LAAP K_d can be used to approximate K_d for aquifer soils. For surface soil, an average value for initial approximations is 5.76 L/kg.

Disappearance Coefficients

Processes that remove explosives contaminants from solution can be approximated with first-order kinetics which take the form

$$dc/dt = -kc \quad (3)$$

where

c = chemical concentration of the reacting substance milograms/liter

k = first order reaction constant, hr^{-1}

t = time, hr

First-order kinetics reduce to the equation

$$\ln (c_0/c) = kt \quad (4)$$

where

c_0 = concentration of the reacting substance at time 0

Once a value of k is obtained, the half-life period of the reacting substance, $t_{1/2}$, can be calculated using the equation.

$$t_{\frac{1}{2}} = 0.693/k \quad (5)$$

Equation 4 has generally provided a good fit to the experimental data (Brannon and Myers 1997; Pennington et al. in preparation) and can be used to describe the disappearance of explosives from solution under various environmental conditions. Use of disappearance rate coefficients in modeling is complicated by the proximity of many of the coefficients to zero and the uncertainty that this creates when applying results from short-term bench scale testing to field scale. Use of the disappearance rate coefficients in groundwater models may require adjustment to accurately depict measured groundwater concentrations that reflect field conditions and a longer time frame than is possible with bench scale tests.

TNT

First-order rate coefficients derived from batch tests for the disappearance of TNT and TNT transformation products from aerobic and anaerobic surface soil are presented by Brannon and Myers (1997). First-order disappearance rate coefficents for TNT in LAAP aquifer soils, which ranged from 0.0006 to 0.0014 hr^{-1} (Pennington et al. in preparation), are substantially lower than the value of 0.062 hr^{-1} measured in an anaerobic surface soil (Brannon and Myers 1997). The same holds true for TNT transformation products in anaerobic and aerobic LAAP aquifer soils (Table 5).

RDX

First-order rate coefficients for the disappearance of RDX from surface soil, which were derived from batch tests under a wide variety of redox potential and pH conditions, have shown that disappearance of RDX is greatest under highly reducing conditions (Table 6). Under most pH conditions at oxidized (+500 mV) and mildly reducing (+250 mV) conditions, the disappearance rate coefficients for RDX could not be differentiated from zero. This indicates that under all but the most highly reducing conditions, RDX will be relatively stable in soils or sediments. Disappearance rates of RDX in LAAP aquifer soils were lower than disappearance rates in surface soils under aerobic and mildly reducing conditions (Table 6).

HMX

HMX is relatively stable under a wide variety of environmental conditions (Table 6). The highest disappearance rate coefficient reported for HMX was 0.06 hr^{-1} in highly reducing surface soil (Price, Brannon, and Hayes 1997). Under most environmental conditions, HMX was relatively stable and was not lost from solution in appreciable amounts.

Photodegradation

Photolysis of explosives occurs in surface waters and on surface soils where the contaminant is exposed to sunlight. Existing rates for photolysis of explosives are summarized in McGrath (1995) and Townsend and Myers (1996). Two major competing pathways appear to degrade TNT. One pathway generates TNB and other intermediate oxidation compounds, whereas the other pathway generates 4A-DNT, 2A-DNT and other reduction intermediates such as 2,6-DANT and 2,4DANT. When explosives are exposed to both photodegradation and biotic plus abiotic soil and sediment processes, the question arises as to which will predominate in the fate and transport of the explosive contaminant. This question is especially relevant for TNT, which is subject to rapid biotic and abiotic transformations under a wide range of

environmental conditions (Price, Brannon, and Hayes 1997; Brannon, Price, and Hayes 1998). Research (Appendix A) has shown that TNT disappearance and transformation in water/soil exposures (water overlying settled soil and suspended soil) were affected by the type of soil exposure but were not appreciably affected by dark and light exposures. These results indicate that processes such as adsorption, sequestration, and biotic and abiotic transformation of TNT rather than photodegradation are the dominant processes in aquatic conditions and will be the major factors affecting disappearance rate and transformation.

5 Conclusions

Conceptual models for UXO fate and transport were developed for the upland and aquatic environments. The state of development for explosives release mechanisms and process descriptor formulations for fate and transport of explosives from UXO were investigated, and important data gaps were identified. The most extensive data gaps are associated with the source term, which encompasses the movement of explosives from UXO into the environment. The source term is strongly affected by UXO integrity, munition type, and the environment in which the munition resides. For a cracked or corroded munition, dissolution rate of the explosive in the munition is one of the more important parameters affecting the fate and transport of the explosive into the environment. Recent research has shown that zero-valent iron greatly reduces explosives concentrations in water, a process that should be active when explosives exit corroded UXO and enter the environment. Adsorption of TNT and RDX by soils can be estimated based on soil CEC. Adsorption of HMX can not now be estimated based on soil physical characteristics. Research was also conducted to explore the relationship between HMX adsorption and soil physical characteristics and the effects of light on TNT disappearance from aquatic systems. Disappearance of TNT from soil/water systems are not appreciably affected by exposure to light. This demonstrates that processes which act independently of light are most important in a soil/water system and will control the disappearance of TNT.

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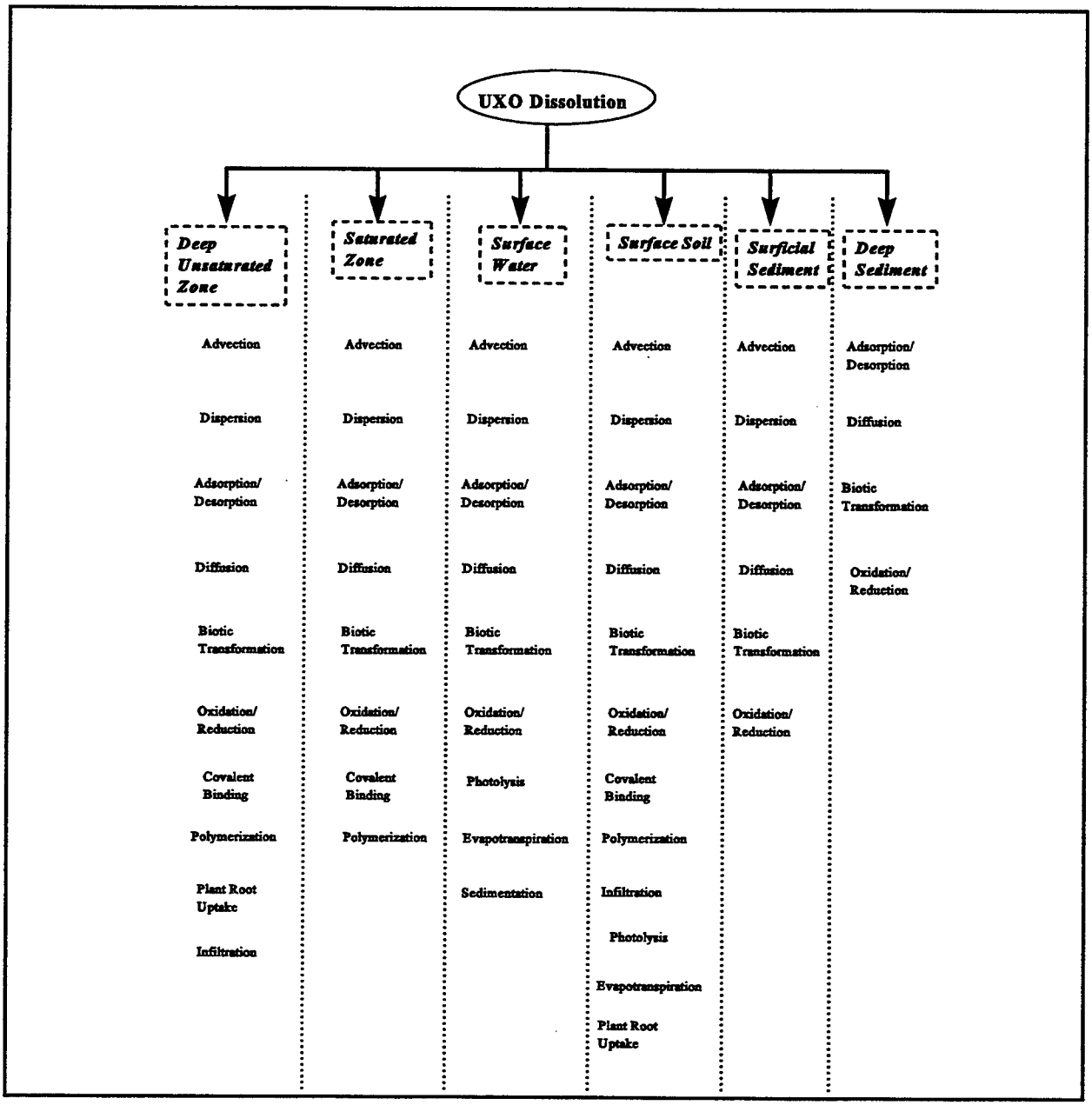

Figure 1. UXO fate and transport processes active in the applicable environments

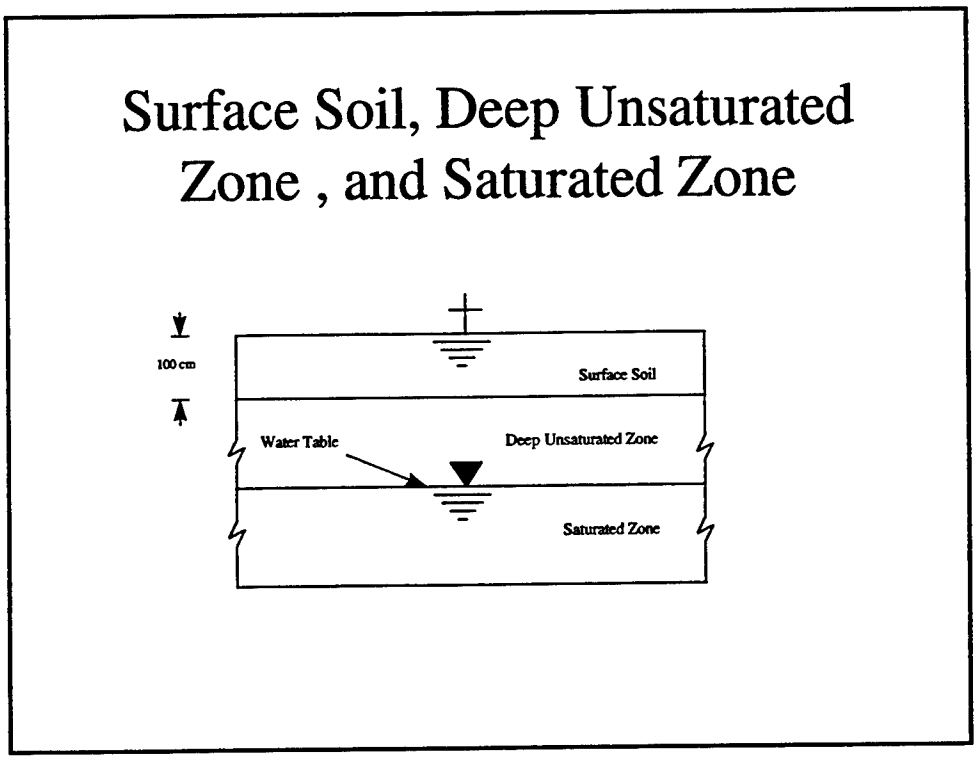

Figure 2. Diagram of the various soil zones

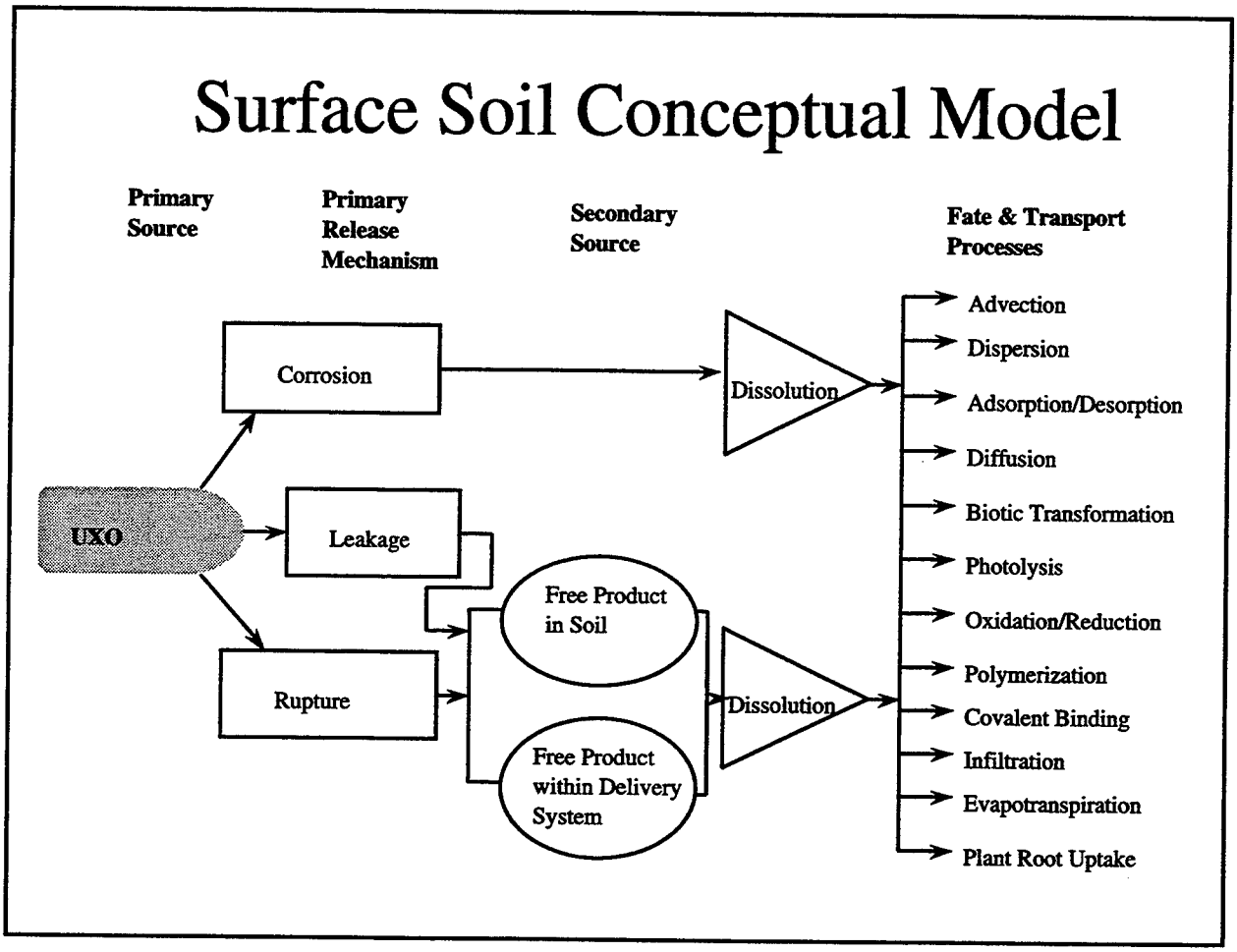

Figure 3. Surface soil conceptual model

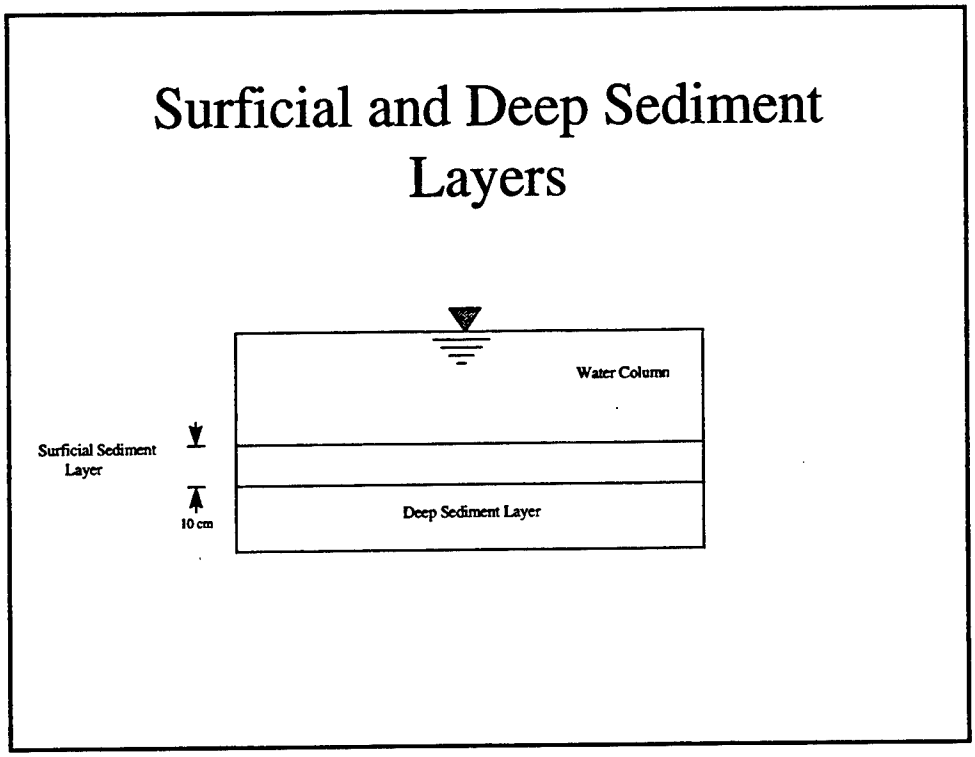

Figure 4. Diagram of surficial and deep sediment layers

Table 1
Dissolution Rate of TNT, HMX, and RDX in a Completely Mixed Aqueous System Derived from Aqueous Concentration Changes over Time[1]

Compound	Rate, $\mu g\ cm^{-2}\ hr^{-1}$	r^2
TNT	4,164	0.986
HMX	702	0.964
RDX	361	0.993

[1] Jenkins and Miyares, unpublished data.

Table 2
Summary of Literature Data Relating K_d of TNT to Soil Properties

Soil	K_d, l/kg	CEC[1], mmol/g	TOC[2], %	Clay, %	Reference
LAAP[3] ML	0.04	3.5	0.015	5	Pennington et al. (in preparation)
LAAP SP-SM	0.09	3.6	0.015	5	Pennington et al. (in preparation)
LAAP CL	0.27	8.1	0.162	15	Pennington et al. (in preparation)
LAAP SM	0.17	5.5	0.02	7.5	Pennington et al. (in preparation)
Norborne C	1.24	9.14	0.23	13	Ainsworth et al. (1993)
Cloudland C	0.81	5.6	0.05	30	Ainsworth et al. (1993)
Westmoreland B1	0.58	6.9	0.98	13.6	Ainsworth et al. (1993)
Ocala C4	4.3	33.5	0.08	33	Ainsworth et al. (1993)
Burbank Ap	1.04	5.5	0.5	4	Ainsworth et al. (1993)
Sand	0.47	1.73	0.36	2.5	Brannon et al. (1992)
Silt	2.23	73	0.96	6.3	Brannon et al. (1992)
Kolin Soil	2.66	16.3	0.18	10.6	Xue, Iskandar, and Selim (1995)
Norwood Soil	3.64	4.1	0.32	3	Xue, Iskandar, and Selim (1995)
Cornhuskers	4.1	35.3	0.83	20	Pennington and Patrick (1990)
Crane	3.7	31.2	2.8	20.6	Pennington and Patrick (1990)
Holston A	4.4	28.8	2.7	18.1	Pennington and Patrick (1990)
Holston B	3.0	35.2	1.2	43.8	Pennington and Patrick (1990)
Iowa	5.2	44.7	1.4	20	Pennington and Patrick (1990)
Joliet	6.8	102	3.6	23.8	Pennington and Patrick (1990)
Kansas	5.7	130.4	2.6	26.3	Pennington and Patrick (1990)
Lonestar	2.5	15.5	0.56	10	Pennington and Patrick (1990)
Longhorn	3.7	20.9	0.56	15	Pennington and Patrick (1990)
Louisiana	2.5	16.3	0.37	10.6	Pennington and Patrick (1990)
Newport	2.3	13.4	3.5	5.6	Pennington and Patrick (1990)
Radford	3.2	21.5	1.1	25	Pennington and Patrick (1990)
Savanna	2.5	13.2	1.3	5	Pennington and Patrick (1990)
Volunteer	4.05	46.4	1.7	5	Pennington and Patrick (1990)
Clay	11	124.9	2.4	54.4	Pennington and Patrick (1990)
Silt	2.8	17.2	0.57	17.5	Pennington and Patrick (1990)

[1] Cation Exchange Capacity.
[2] Total Organic Carbon.
[3] Louisiana Army Ammunition Plant.

Table 3
Summary of Literature Data Relating K_d of RDX to Soil Properties

Soil	K_d, l/kg	CEC [1], mmol/g	TOC [2], %	Clay, %	Reference
LAAP [3] ML	0.21	3.5	0.015	5	Pennington et al. (In preparation)
LAAP SP-SM	0.33	3.6	0.015	5	Pennington et al. (In preparation)
LAAP CL	0.33	8.1	0.162	15	Pennington et al. (In preparation)
LAAP SM	0.33	5.5	0.02	7.5	Pennington et al. (In preparation)
Elk-B1	0.27	6.92	0.45	16.5	Ainsworth et al. (1993)
Cloudland C	0.12	5.6	0.05	30	Ainsworth et al. (1993)
Cecil AP	0.43	4.88	0.59	62	Ainsworth et al. (1993)
Cecil BT	0.31	2.92	0.32	53	Ainsworth et al. (1993)
Burbank Ap	0.16	5.5	0.5	4	Ainsworth et al. (1993)
Kenoma BC	0.93	31.4	0.5	44	Ainsworth et al. (1993)
Kenoma Bt1	1.21	26	1.43	44	Ainsworth et al. (1993)
Ocala C4	2.37	33.5	0.08	33	Ainsworth et al. (1993)
Watson 2Bxg	1.45	10.3	0.4	47	Ainsworth et al. (1993)
Westmoreland A1	1.65	6.91	2.03	14.4	Ainsworth et al. (1993)
Sand	0.29	1.73	0.36	2.5	Brannon et al. (1992)
Silt	1.20	73	0.96	6.3	Brannon et al. (1992)
Rathbun (Extracted)	8.4	114	0.92	16.5	Brannon et al. (1992)
Kolin Soil	1.59	16.3	0.18	10.6	Xue, Iskandar, Selim (1995)
Norwood Soil	1.57	4.1	0.32	3	Xue, Iskandar, Selim (1995)
Yokena Clay	3.5	38.9	2.4	48.7	Brannon, unpublished data
West End	2.2	45.7	0.18	7.5	Brannon, unpublished data
Yuma	1.07	5.4	0.04	5.0	Brannon, unpublished data
D Street	0.82	1.8	0.17	0.0	Brannon, unpublished data

[1] Cation Exchange Capacity.
[2] Total Organic Carbon.
[3] Louisiana Army Ammunition Plant.

Table 4
Summary of Literature Data Relating K_d of HMX to Soil Properties

Soil	K_d, l/kg	CEC [1], mmol/g	TOC [2], %	Clay, %	Reference
LAAP [3] ML	0.086	3.5	0.015	5	Pennington et al. (in preparation)
LAAP SP-SM	0.20	3.6	0.015	5	Pennington et al. (in preparation)
LAAP CL	0.37	8.1	0.162	15	Pennington et al. (in preparation)
LAAP SM	0.20	5.5	0.02	7.5	Pennington et al. (in preparation)
Browns Lake	7.42	15.3	0.38	10.0	This study (Appendix A, Table A1)
Montmorillonite	4.99	13.2	0.19	30	This study (Appendix A, Table A1)
Yokena Clay	12.1	38.9	2.40	48.8	This study (Appendix A, Table A1)
St. Mary Parish, LA	17.7	14.2	0.19	20	This study (Appendix A, Table A1)
Picatinny B	4.25	9.8	0.634	5	This study (Appendix A, Table A1)
Socorro S	3.25	34.0	0.08	35	This study (Appendix A, Table A1)
Socorro P	1.17	27.3	0.12	27.5	This study (Appendix A, Table A1)
Grange Hall Silt	0.12	16.7	0.29	10	This study (Appendix A, Table A1)
Yuma 1B	5.02	8.6	0.03	5	This study (Appendix A, Table A1)
China Lake	1.65	3.5	0.02	5	This study (Appendix A, Table A1)

[1] Cation Exchange Capacity.
[2] Total Organic Carbon.
[3] Louisiana Army Ammunition Plant.

Table 5
Kinetics (K^{-1}, hr^{-1}) for TNT and its Transformation Products with Two LAAP Aquifer Soils under Aerobic and Anaerobic Conditions Following Addition of 100 mg/l of the Respective Compounds (Pennington et al. in preparation)

	SP-SM Soil, anaerobic			SP-SM Soil, aerobic			SM Soil, anaerobic			SM Soil, aerobic		
Compound	r^2	K^{-1}, hr^{-1}	$t_{1/2}$, hr	r^2	K^{-1}, hr^{-1}	$t_{1/2}$, hr	r^2	K^{-1}, hr^{-1}	$t_{1/2}$, hr	r^2	K^{-1}, hr^{-1}	$t_{1/2}$, hr
TNT	0.43	-0.00064	SD[1]	0.19	0.001	NS[2]	0.31	0.0016	433	0.73	0.0025	282
4ADNT	0.85	-0.0045	SD[1]	0.44	0.0026	267	0.88	-0.0059	SD[1]	0.56	0.032	21
2ADNT	0.88	-0.0052	SD[1]	0.59	0.0028	244	0.74	-0.004	SD[1]	0.46	0.0022	320
2,4DANT	0.78	0.0094	74	0.95	0.0008	826	0.79	0.0094	74	0.96	0.006	115
2,6DANT	0.22	0.0032	NS[1]	0.80	0.0006	1,246	0.85	0.0068	101	0.94	0.004	173

[1] SD = Rate constant is significantly ($p < 0.5$) different from zero, but concentrations increased over time, resulting in an indeterminate half-life.
[2] NS = Rate constant is not significantly ($p < 0.5$) different from zero.

Table 6
First-Order Disappearance Rate Coefficients (K^{-1}, hr^{-1}) for RDX and HMX

Soil Type and Conditions	Explosive Compound	K^{-1}, hr^{-1}	Source
Surface soil, oxidizing conditions	RDX	0 - 0.007	Price, Brannon, and Hayes (1997)
Surface soil, mildly reducing conditions	RDX	0 -0.008	Price, Brannon, and Hayes (1997)
Surface soil, highly reducing conditions	RDX	0.16 - 0.24	Price, Brannon, and Hayes (1997)
Aquifer soils	RDX	0 -0.0003	Pennington et al. (1997)
Surface soil, oxidizing conditions	HMX	0	Price, Brannon, and Hayes (1997)
Surface soil, mildly reducing conditions	HMX	0	Price, Brannon, and Hayes (1997)
Surface soil, highly reducing conditions	HMX	0 - 0.06	Price, Brannon, and Hayes (1997)
Aquifer soils	HMX	0 - 0.0004	Pennington et al. (1997)

Appendix A
HMX Adsorption and TNT Photodegradation

Introduction

Development of equations for prediction of HMX K_d from soil properties requires empirical measurements of K_d on well characterized soils. Such measurements were unavailable. Therefore, one objective of the study was to conduct additional adsorption testing with HMX using soils of known physical and chemical characteristics to expand the inadequate available data on HMX adsorption.

The fate of explosives in the aquatic environment will be affected by sorption, transformation, and photodegradation. However, the relative significance of sorption and transformation processes compared to photodegradation is unknown for the two most common aquatic situations, water and suspended soil, and water overlying settled soil. This is important for modeling the fate and transport of explosives in the aquatic environment because more data are available on sorption and transformation in soil/water systems than is available for photodegradation. Therefore, the second objective of the study was to determine if photodegradation or sorption and transformation processes mediated by suspended and settled soils are the dominant processes for TNT in aquatic systems.

Materials and Methods

HMX adsorption

Batch adsorption isotherm tests were conducted at 20 °C on 10 soils possessing a wide range of physicochemical characteristics such as cation exchange capacity (3.5 to 38.9 meq/100g) and total organic carbon (0.02 to 2.4 percent) (Table A1). To triplicate 250-ml glass centrifuge tubes, 4 gm oven dry weight of each of the soils and 16 ml of distilled-deionized water were

loaded. The samples were then spiked with radiolabeled HMX[1] at five different concentrations (0.1, 0.3, 0.5, 0.8 and 1 ug/g soil dry weight). After spiking, the tubes were shaken for 24 hr on a reciprocating shaker, centrifuged for 1 hr at 7,400 relative centrifugal force, and sampled by removing 1 ml. The sample was counted in a Packard TriCarb 2500 Liquid Scintillation Analyzer (Packard Instruments Inc., Meriden, CT).

TNT photodegradation

Soil collection. Yokena clay (49 percent clay), an agricultural surface soil from the Mississippi River floodplain, was used. The soil was classified as very fine, montmorillonite, nonacid, thermic Vertic Haplaquept (Natural Resources Conservation Service classification) and designated Yokena clay. The soil was air-dried, ground, and sieved through a 2-mm (0.08-in.) sieve. The sieved samples were thoroughly mixed, transferred to polyethelene containers, sealed, and stored at room temperature.

Treatments

Water only. To measure photodegradation without the effects of soil, water-only treatments were conducted in 3-l Griffin beakers containing 2 l of distilled water maintained at room temperature (25 °C). The beakers were positioned at random directly under the light sources to eliminate container interference or in the dark and stirred with a magnetic stirrer. Light sources consisted of full-spectrum fluorescent lights (20 μ Einsteins (ϵ) /m^2/sec intensity) (low-light intensity) or Lumalux high-pressure sodium lamps and Metalarc metal halide lamps (General Electric Company, Fairfield, CT) with a combined intensity of 367 μϵ/m^2/sec (high-light intensity). For the dark control, the beakers were wrapped in aluminum foil and a felt curtain was placed over the experimental apparatus to block out any light. The dark- and low-light intensity tests were conducted in triplicate and the high-light intensity tests were not replicated because of the close agreement between replicates observed for the low-light experiments. Each test was spiked with 0.03 g of TNT in 2 ml of methanol, sufficient TNT to obtain a final solution concentration of 15 mg TNT/liter. Twenty-ml samples were withdrawn from each test following the spiking at intervals of 5, 15, 30 min, 1, 4, 24, 72, and 168 hr. Samples were immediately frozen until analyzed (see chemical analyses below).

Suspended soil. To determine the effects of suspended soil on photodegradation, suspended soil treatments were conducted in the same manner as the water-only treatment except that Yokena Clay was added to each beaker to produce a slurry concentration of 500 mg suspended soil/liter of water. The soil

[1] HMX was uniformly ring labeled [(U-^{14}C) HMX] (New England Nuclear Research Products, Boston, Massachusetts) having a specific activity of 8.2 mCi/mmol with a radiochemical purity of 97 percent.

was kept in suspension by magnetic stirrers. Each test was spiked with a final solution concentration of 15 mg TNT/liter of suspension. Twenty-ml samples were withdrawn from each test at intervals of 5, 15, 30 min, 1, 4, 24, 72, and 168 hr. Sampling quantity and intervals were the same as for the water-only treatment except that the samples were centrifuged at 7,400 RCF for 20 min in 25-ml glass centrifuge tubes to separate the aqueous and solid phases. The aqueous phase was frozen until analyzed.

Overlying water. To determine the effects of settled soil on photodegradation, settled soil experiments (overlying water treatments) were conducted. Distilled-deionized water (2,500 ml) was poured over 775 g Yokena clay and allowed to incubate for 2 weeks to develop anaerobic conditions in the settled soil before testing. The overlying water was removed and replaced with 2 l of fresh distilled-deionized water and stirred gently using Arrow-6000 overhead stirrers. Each test was spiked to a final solution concentration of 15 mg TNT/liter. Light and dark exposures were conducted as described for the water-only exposures. Sampling and sample analyses were identical to those for the suspended soil treatment.

Radioassay. To determine the effects of treatments on extractability of TNT, water-only, suspended soil, and overlying water treatments were conducted as previously described except that tests were spiked with ^{14}C labeled TNT.[1] The spike consisted of 99 parts unlabeled TNT and 1 part radiolabeled TNT. Aqueous phase samples were counted in a Packard TriCarb 2500 Liquid Scintillation Analyzer (Packard Instruments, Inc., Meriden, CT).

Chemical analyses

Aqueous phase concentrations of TNT and the transformation products 1,3,5-trinitrobenzene (TNB), 1,3-dinitrobenzene (DNB), 2,6-dinitrotoluene (2,6DNT), 2,4-dinitrotoluene (2,4DNT), 4-amino-2,6-dinitrotoluene (4A-DNT), 2-amino-4,6-dinitrotoluene (2A-DNT), 3,5-dinitroanaline (DNA), 2,6-diamino-4-nitrotoluene(2,6-DANT), and 2,4-diamino-6-nitrotoluene (2,4-DANT) were analyzed by HPLC using a Supelco LC-18 reverse phase column, a Supelco LC-CN reverse phase confirmatory column, and a 50-percent methanol:50-percent reagent grade water mobile phase as described by EPA 846 Method 8330 (U.S. Environmental Protection Agency 1995).[2] The compounds 4,4',6,6'-tetranitro-2,2'-azoxytoluene and 2,2',6,6'-tetranitro-4,4'azoxytoluene were analyzed by HPLC using the same methods as for the other explosives except that a 54-percent acetonitrile:46-percent reagent grade water mobile phase was used.

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[1] TNT was uniformly ring labeled [U-^{14}C] (Chemsyn Science Laboratories, Lenexa, Kansas) having a specific activity of 21.58 mCi/mmol, a chemical purity > 98 percent as determined by high-performance liquid chromatography (HPLC), and a radio chemical purity >98 percent as determined by radio-HPLC.

[2] References are listed following main test.

Results and Discussion

HMX adsorption

Linear adsorption isotherms described the sorption of HMX by soils, displaying values of r^2 between 0.88 and 0.99 (Table A2). Only 3 of the 10 regression lines were below an r^2 value of 0.90. HMX adsorption coefficients ranged from 0.12 l/kilogram to 17.7 l/kilogram for the 10 soils.

Photodegradation

TNT disappearance. In the water-only treatment, concentrations of TNT in the light and dark treatments did not differ significantly (Figure A1) and no significant decrease in TNT concentrations was observed. This agrees with the findings of Kocharny and Bolton (1992), who reported that light alone is not sufficient to significantly affect TNT concentrations in water. However, decreases in TNT concentrations were observed in the overlying water and suspended soil treatments even though differences between light and dark exposures were minimal (Figure A1). The rate of TNT disappearance was more rapid in the overlying water treatment than in the suspended sediment treatment. The limited sensitivity to light should not be due to the lack of appropriate quantized energies in the fluorescent light source. Treatments with higher-intensity, full-spectrum lights (367 $\mu\epsilon/m^2/sec$) that simulate sunlight (Lumalux high-pressure sodium lamps and Metalarc metal halide lamps) gave results similar to the lower-intensity (20 $\mu\epsilon/m^2/sec$) fluorescent light source.

The lack of TNT concentration differences between light and dark exposures within a treatment indicates that factors such as biodegradation, sequestration, and/or adsorption affect TNT concentrations to a much greater extent than photolysis. Adsorption of TNT and its degradation products was occurring, as shown by aqueous phase ^{14}C results (Figure A2). Recoveries following 7 days of testing showed that adsorption was higher in the overlying water treatment, but that recoveries of radioactivity within a treatment were roughly comparable.

TNT transformation products. Formation of TNT transformation products in the water-only treatment was limited to TNB (Figure A3). Concentrations of TNB (although small) in the water-only treatment increased with light intensity. This is probably because formation of TNB is due to an oxidation mechanism, which is more light-dependent than the reduction mechanism responsible for the formation of the other aromatic nitroamines. TNB was also produced in the suspended soil treatment and in the overlying water treatment for a short time (<72 hr). Concentrations of TNB were highest in the high-light intensity exposures. Formation of amino reduction products in the suspended soil treatment was limited to 4A-DNT and 2A-DNT in the high-intensity light treatment (Table A3). The highest concentrations of transformation products were produced in the overlying water treatment, with concentrations of all but TNB present in solution after 3 days of exposure. This is apparently due to the

higher reducing capacity of the settled soil, as indicated by the rapid disappearance TNB from the overlying water, compared to the suspended soil.

The nature and quantity of TNT transformation products indicated the existence of competing oxidation and reduction mechanisms. This resulted in formation of different combinations of transformation products among treatments and in different concentrations within a treatment as a function of light intensity.

Aminonitrotoluenes are most likely formed from TNT by reducing agents and microbes indigenous to the soil. The amounts of TNT transformation products are small compared to the amount of disappearance of TNT (Table A3), which means that TNT disappearance in water/soil systems is controlled more by adsorption and sequestration than by transformation due to either soil processes or photodegradation.

Conclusions. High-quality HMX adsorption coefficients were obtained using soils of known characteristics to allow correlation in the main body of this report. The photodegradation studies showed that TNT concentrations in water and water/soil systems were affected by the presence of soil both in suspension and beneath the water column but were not appreciably affected by dark and light exposures. Recoveries of radioactivity in the aqueous phase showed that adsorption/sequestration was responsible for most observed differences. Light exposures resulted in different transformation products among treatments and in different concentrations of products within a treatment. In the water-only treatment, TNB was the only transformation product produced. In the presence of soil, mono and diamino reduction products were the primary TNT transformation products. These HMX and photodegradation findings will facilitate development of process descriptor formulations in soils and aquatic environments.

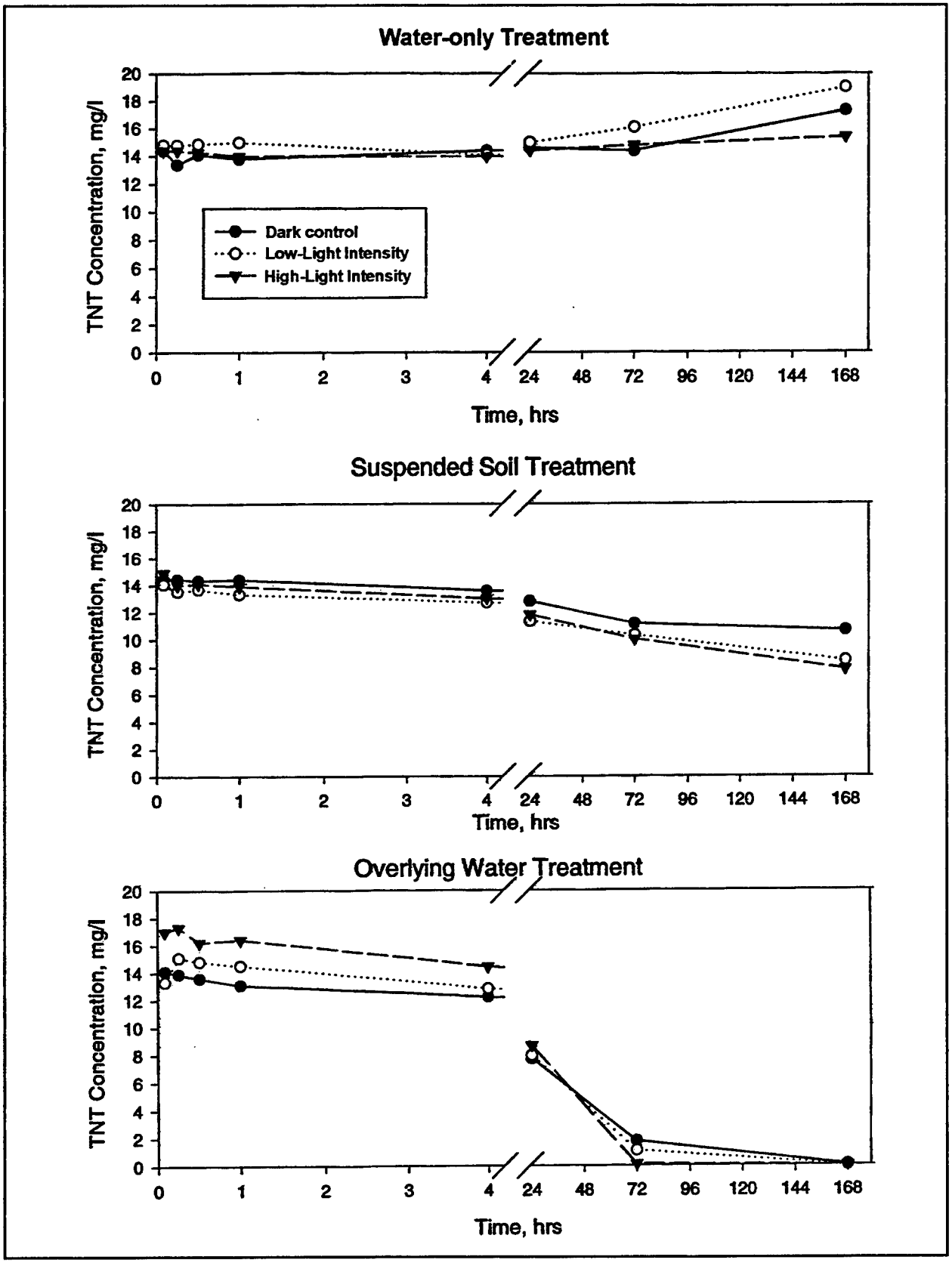

Figure A1. TNT solution concentrations in water and water/soil treatments under different light conditions

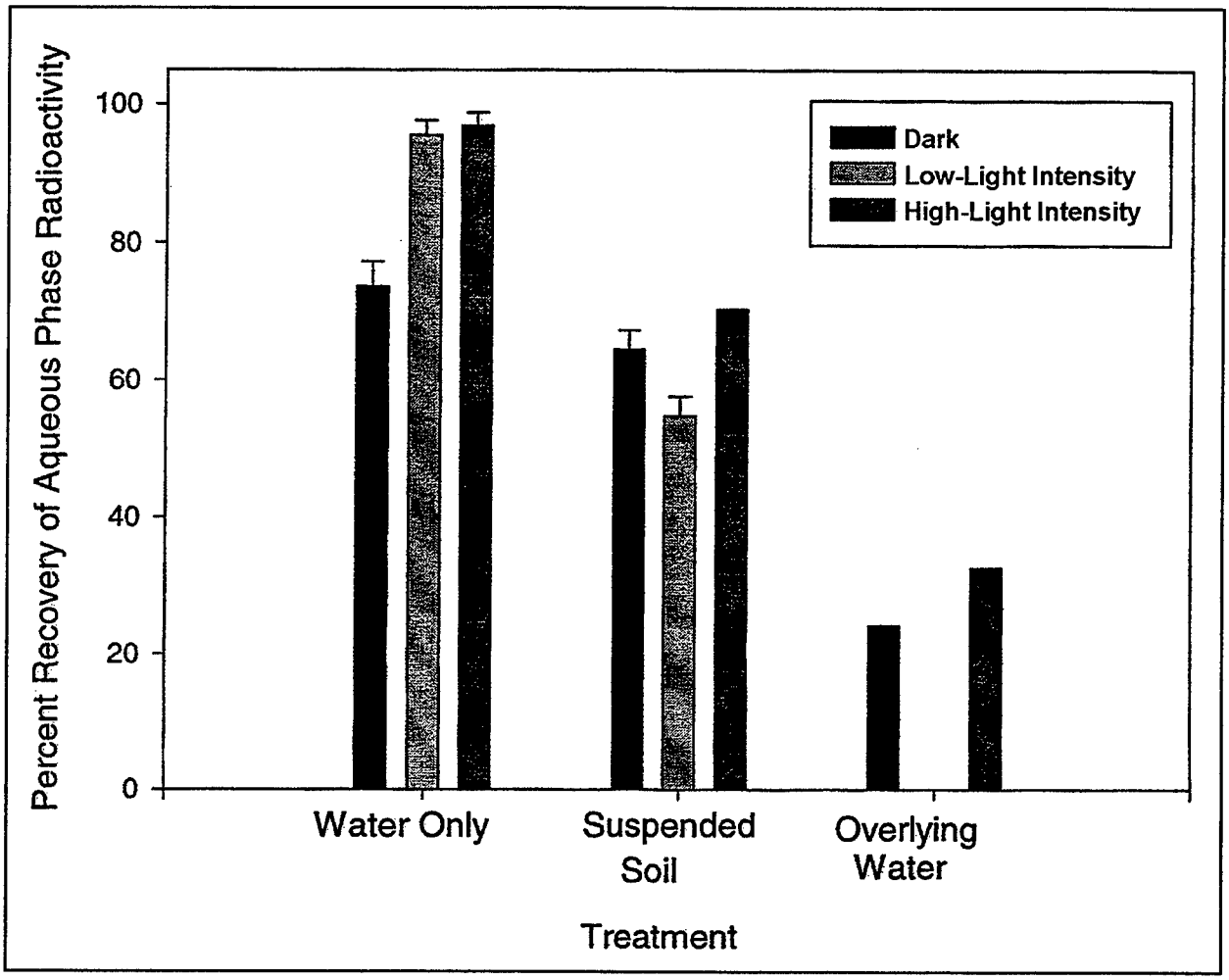

Figure A2. TNT radioisotope solution recovery in the various water/soil treatments under dark, low-light (LL) and high-light (HL) intensity conditions

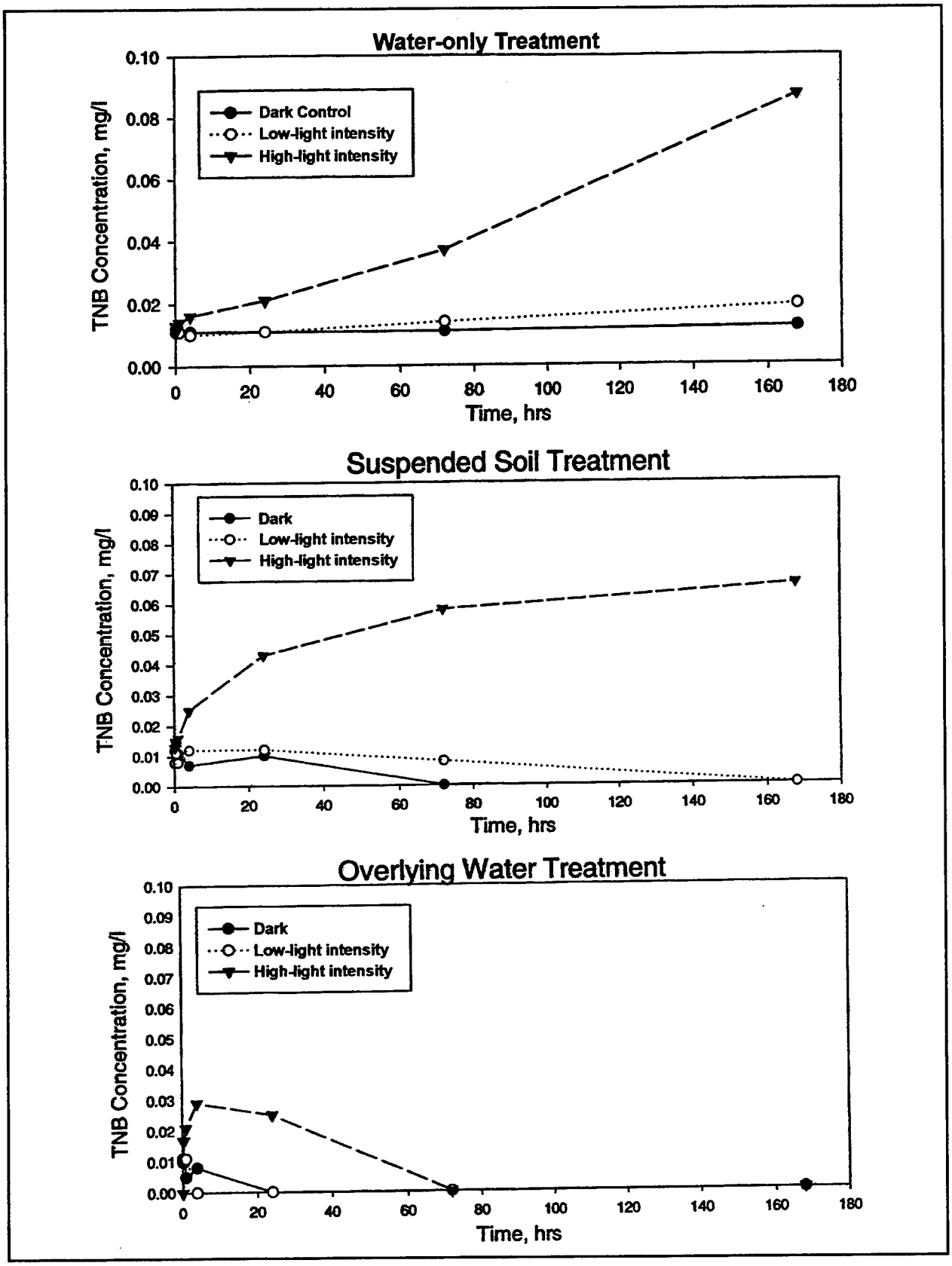

Figure A3. TNB solution concentrations in water and water/soil treatments under different light conditions

Table A1
Physical Characteristics of Soils Used in HMX Adsorption Testing

Soil	Particle Size Distribution			Cation Exchange Capacity, mmol/g	Total Organic Carbon, %
	Sand, %	Silt, %	Clay, %		
Browns Lake	51.0	39.0	10.0	15.3	0.38
Montmorillonite	35	35	30	13.2	0.19
Yokena Clay	13.75	37.5	48.75	38.9	2.40
St. Mary Parish, LA	45	35	20	14.2	0.19
Picatinny B	62.5	32.5	5	9.8	0.634
Socorro S	37.5	35	27.5	34.0	0.08
Socorro P	42.5	30	27.5	27.3	0.12
Grange Hall Silt	39	51	10	16.7	0.29
Yuma 1B	92.5	2.5	5	8.6	0.03
China Lake	92.5	2.5	5	3.5	0.02

Table A2
Adsorption Coefficients (K_d's) and Linear Regression Coefficients (r^2) for HMX Adsorption Isotherms

Soil	K_d l/kg	r^2
Browns Lake	7.42	0.88
Montmorillonite	4.99	0.96
Yokena Clay	12.1	0.89
St. Mary Parish, LA	17.7	0.95
Picatinny B	4.25	0.94
Socorro S	3.25	0.99
Socorro P	1.17	0.95
Grange Hall Silt	0.12	0.93
Yuma 1B	5.02	0.88
China Lake	1.65	0.91

Table A3
Concentrations (mg/l) of TNT Transformation Products Following 3 Days of Incubation

	Water-only Treatment			Suspended Soil Treatment			Overlying Water Treatment		
Compound	Dark	LL	HL	Dark	LL	HL	Dark	LL	HL
2A-DNT	<0.02	<0.02	<0.02	<0.02	<0.02	0.03	0.46	0.59	0.65
4A-DNT	<0.02	<0.02	<0.02	<0.02	<0.02	0.06	0.56	0.74	0.93
2,6-DANT	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.09	0.11	0.12
2,4-DANT	<0.2	<0.2	<0.2	<0.2	<0.2	<0.2	0.4	0.03	0.68
TNB	0.011	0.014	0.04	<0.02	0.008	0.06	<0.02	<0.02	<0.02

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13. ABSTRACT ***(Maximum 200 words)***

Primary release mechanisms for explosives from UXO are identified and conceptual models for UXO fate and transport were developed for the upland and aquatic environments. The state of development for explosives release mechanisms and process descriptor formulations for fate and transport of explosives from UXO were investigated and important data gaps were identified. The most extensive data gaps are associated with source term, which encompasses the movement of explosives from UXO into the environment. The source term is strongly affected by UXO integrity, munition type, and the environment in which the munition resides. For a cracked or corroded munition, dissolution rate of the explosive in the munition is one of the more important parameters affecting the fate and transport of the explosive into the environment. Explosives exiting corroded UXO could be transformed by exposure to iron, a process shown to strongly affect explosives. Adsorption of TNT and RDX by soils can be estimated based on soil cation exchange capacity. Research was also conducted to explore the relationship between HMX adsorption and soil physical characteristics and the affects of light on TNT disappearance from aquatic systems. Disappearance of TNT from soil/water systems is not appreciably affected by exposure to light. This demonstrates that processes which act independently of light are most important in a soil/water system and will control the disappearance of TNT.

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